Plug and Play Approach to Verification and Validation

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One of the most pressing needs in science and engineering is that of developing solid and reliable methods to verify and validate the methods we use to predict the behavior of complex systems. In the present work, we follow the standard nomenclature of terming the process of verification as the task of making sure that the equations of the model are solved correctly and the process of validation as the task of making sure that the model equations represent with fidelity the actual physics of the system under investigation.

We present a new approach for verification and validation (V&V), focusing particularly on the challenging task of validation. The idea we propose is to test validation by going beyond the traditional approach of comparing the results of a model with experiments. The approach proposed here brings validation to a new level because it not only validates the prediction of commonly used models by testing their results, but it also validates models by directly testing the assumptions behind them (e.g., equations of state or closure relations). We validate the assumptions and not just the predictions. Indeed it often happens that models can give falsely right predictions in some cases and fail miserably in others. Or models can be fudged into giving the right answer. We propose a method that goes after the inadequacies in the assumptions behind a given model. We contend this is the only way to achieve a true physics-based predictive capability: we need to make sure the methods we use are solidly based and their assumptions are valid.

We have developed the approach into a new software infrastructure aimed specifically at achieving the goals we set in our new approach. The code project for this effort has been named PARSEK [1] and was a component of the R&D 100-winning CartaBlanca project [2]. The approach is based on using particle-based algorithms to simulate different levels of physical complexity. We consider here heat and mass transfer in a multicomponent plasma at the kinetic and fluid level. We have recently reviewed the issue, providing a general formalism for fluid closures [3]. By representing both the fluid and the kinetic levels using particle methods we have designed a component-based software package to conduct validation using a plug and play approach.

We term the new approach “plug and play validation” [4] because it allows us to validate coarser levels of description with finer levels of description by plugging in components and testing them in use. With the plug and play paradigm, different components representing different physical descriptions but all based on a common particle algorithm can be interchanged without altering the overall software architecture and the overall algorithm. The advantage of the plug and play approach is that validation can be conducted for each component and switching between physical descriptions requires the validation of just the affected components, not entire codes. Verification is also greatly simplified as all components share the same software infrastructure.

We present one paradigmatic application of the plug and play approach to the study of fluid modeling of electron holes created by the two-stream instability in relativistic plasmas. Figure 1 shows the evolution of the distribution function of the electrons in a plasma at high energy (10 MeV) with ultrarelativistic velocities. The plasma is initially characterized by two counter-streaming electron populations, typically obtained in the laboratory and in astrophysics by shock acceleration or compression. Many of the fluid models typically used [3] would predict that the system is stable and no heat flux or temperature gradient is present. We have applied our new plug and play V&V approach, and we have demonstrated the failure of many fluid closures described in the literature [4]. Figure 1 shows the kinetic evolution of the two electron populations. Figure 2 shows a comparison of the fine description (kinetic) with the coarse (fluid) description. The fluid moments are computed directly from the kinetic model and the validity (or failure of it) of fluid models is tested directly [5].

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[2] N.T. Padial-Collins, et al., *Concurrency and Computation: Practice and Experience* **16** (1), 61–77 (2004).
[3] L. Abrardi, et al., "Kinetic Theory of a Gas Mixture Far from Thermodynamic Equilibrium : Derivation of the Transport Coefficents," Los Alamos National Laboratory report LA-UR-03-8334 (November 2003).
[4] G. Lapenta and S. Markidis, *Lecture Notes in Computer Science* **3516,** 88 (2005).
[5] G. Lapenta, S. Markidis, A. Marocchino, "What is the Origin of Power Laws?" *Nature*, submitted.

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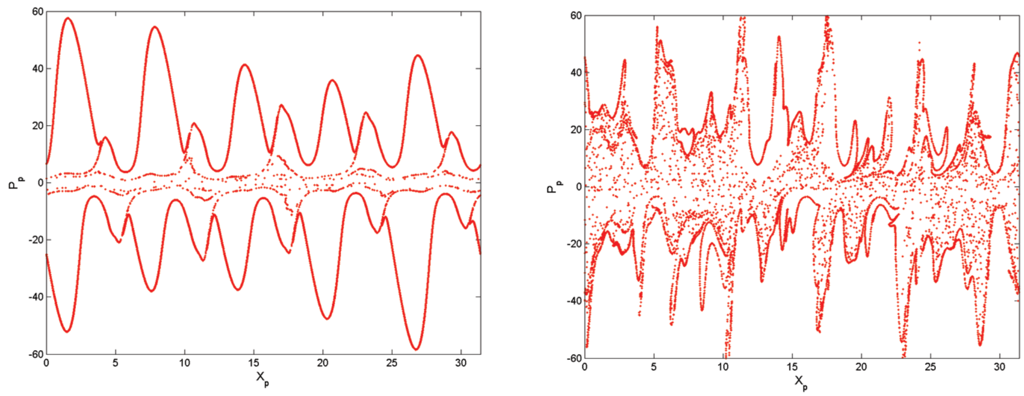

Fig. 1.
Particle plot in phase space for a relativistic plasma during different stages of evolution of the two-stream instability. The early phase is evident on the left where the initial beams are still evident and thermalization is starting. On the right a fully developed nonlinear state is shown, still showing a memory of the initial state, a condition difficult to represent in common fluid models.

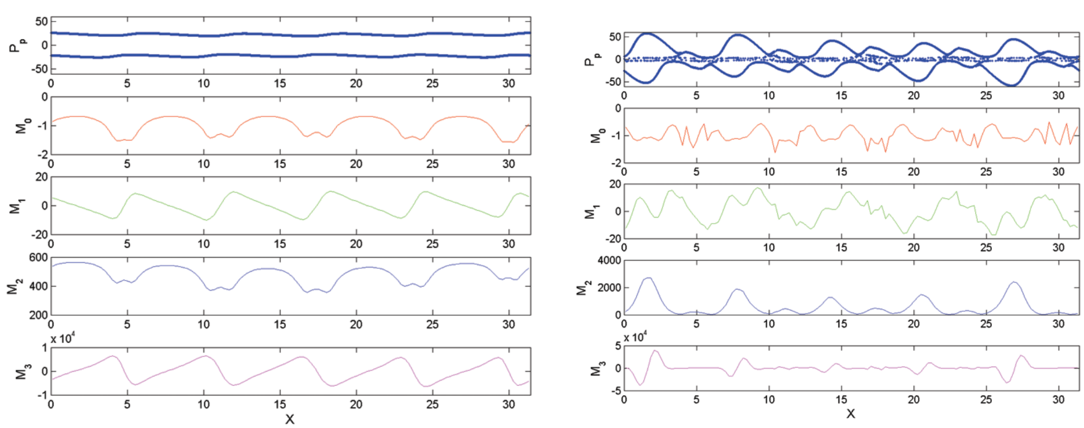

Fig. 2.
Moments of the distribution. The phase space is reported on top for reference. The subsequent panels show charge density, average velocity, temperature, and heat flux. Two different stages of the evolution are shown, an early stage on the left, a later stage on the right. In all cases the heat flux is important and completely missed by simple-minded fluid closure models. Electron holes observed in experiments are evident and the role of heat flux in them is dominant.